

## Heat Conduction in Ceramic Coatings: Relationship between Microstructure and Effective Thermal Conductivity

### Technical report for Task 1

(period of performance Nov. 7, 1996 - Feb. 6, 1997)

Contract Number: NAS3-97002

016743

Research on the effective thermal conductivity of ceramic coatings and its relation to the microstructure continued. Experimental data on thermal conductivity of ceramic coatings provided by NASA (paper by R. Miller *et al* "The effect of plasma spray parameters on density, cyclic life and thermal conductivity of a  $\text{ZrO}_2\text{-Y}_2\text{O}_3$  thermal barrier coatings", Presented at the *ASM-AIME/ Materials Week*, Cleveland, Ohio, October 1995) indicates the necessity of construction a theoretical framework for the analysis of anisotropic conductivity in terms of the microstructural parameters. Our effort was focused on this task.

We employed the approach similar to the one developed earlier for effective elastic properties of materials with defects and developed it further for the thermal conductivity problem. We started with the analysis of the influence of one pore on the overall heat flux. This influence is strongly dependent on the shape of the pore. We model pores as full insulators (this modelling can be viewed as the first approximation and can later be refined to account for a finite, albeit small, conductivity of a pore).

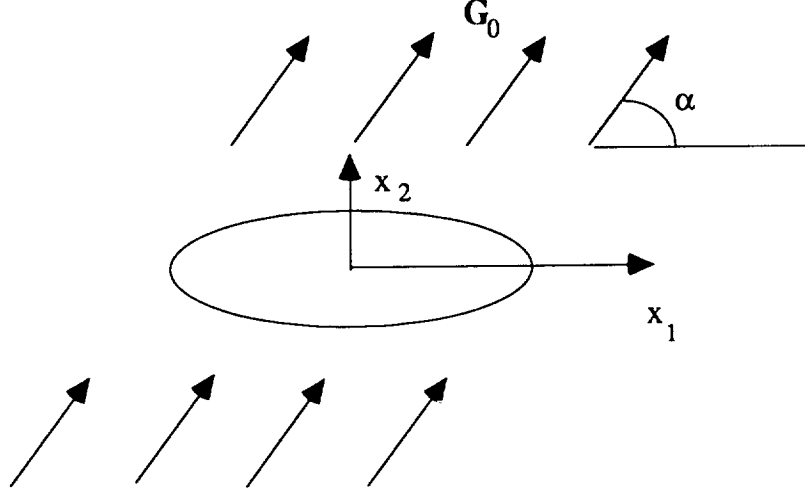
We first analyzed pores of *elliptical* shapes. Such shapes, although simple, constitute an important example: they demonstrate the importance of shape factors. Also, they cover both cracks and circles as limiting cases, and allow one to consider the practically important case of mixtures of cracks/pores. We start with the analysis of an influence of one such pore on the overall heat flux. A summary of our findings is as follows.

One elliptical hole. We consider a 2-D infinite medium of thermal conductivity  $k_0$  with an insulating ( $k = 0$ ) elliptical inclusion (axes  $2a$  and  $2b$ ). The heat flux vector  $\mathbf{Q}_0 = k_0 \mathbf{G}_0$  far away from the inclusion is inclined at an angle  $\alpha$  to the major semi-axis of the ellipse.

The scalar potential  $\Omega$  on the contour of the elliptical inclusion is

$$\Omega = -k_0 G_0 (a + b) \cos(\theta + \alpha) \quad (1)$$

where  $\theta$  is angular elliptical coordinate of the point on the boundary of an inclusion, as given by conformal mapping  $z = R(m\xi + 1/\xi)$ ,  $\xi = e^{i\theta}$ ,  $R = (a+b)/2$ ,  $m = (a-b)/(a+b)$ .



The macroscopic heat flux for the representative area element (RAE) containing a hole is:

$$Q \equiv \frac{1}{A} \int_{\Gamma} \Omega n d\Gamma = \frac{1}{A} \int_{A_s} Q dA - \frac{1}{A} \int_{\gamma} \Omega n d\Gamma \equiv Q_0 + \Delta Q \quad (2)$$

where  $A$  - representative area,  $\gamma$  - hole boundary,  $A_s$  - area of the solid phase and  $\Omega(G_1, G_2)$  is a scalar potential such that  $Q_1 = \frac{\partial \Omega}{\partial G_1}$ ,  $Q_2 = \frac{\partial \Omega}{\partial G_2}$ .

In the case of the elliptical hole, our calculations yield

$$n_1 = \frac{(m-1)\cos\theta}{\sqrt{1+m^2-2m\cos 2\theta}}, \quad n_2 = \frac{(m+1)\sin\theta}{\sqrt{1+m^2-2m\cos 2\theta}}, \quad d\Gamma = R\sqrt{1+m^2-2m\cos 2\theta} d\theta \quad (3)$$

$$\Delta Q_1 = -\frac{k_0 G_0}{A} \pi b(a+b) \cos \alpha = -\frac{k_0}{A} \pi b(a+b) G_1 \quad (4)$$

$$\Delta Q_2 = -\frac{k_0 G_0}{A} \pi b(a+b) \sin \alpha = -\frac{k_0}{A} \pi b(a+b) G_2 \quad (5)$$

Thus, the heat flux change  $\Delta Q$  can be represented as  $\Delta Q = \mathbf{H} \cdot \mathbf{G}$  where  $\mathbf{H}$  is the following second rank tensor:

$$\mathbf{H} = -\frac{k_0}{A} \pi(a+b)(b\mathbf{e}_1\mathbf{e}_1 + a\mathbf{e}_2\mathbf{e}_2) = -\frac{k_0}{A} \pi(ab\mathbf{I} + a^2\mathbf{e}_2\mathbf{e}_2 + b^2\mathbf{e}_1\mathbf{e}_1) \quad (6)$$

The additional (due to the hole) heat energy potential  $\Delta\Omega$  is expressed in terms of tensor  $\mathbf{H}$ :

$$\Delta\Omega = \frac{1}{2} \mathbf{G} \cdot \mathbf{H} \cdot \mathbf{G} \quad (7)$$

In the case of many holes, we first consider the approximation of non-interacting holes: we assume that each hole experiences the influence of the same far-field temperature gradient  $\mathbf{G}$  unperturbed by the presence of the other holes. Then,

$$\mathbf{H} = \sum \mathbf{H}^{(i)} = -\frac{k_0}{A} \pi \left[ \sum a^{(i)} b^{(i)} \mathbf{I} + \sum (a^2 \mathbf{nn} + b^2 \mathbf{mm})^{(i)} \right] = -k_0(p\mathbf{I} + \boldsymbol{\beta}) \quad (8)$$

where  $\mathbf{m}^{(i)}$  and  $\mathbf{n}^{(i)}$  are the unit vectors aligned with the semi-axes ( $a^{(i)}$  and  $b^{(i)}$ , correspondingly) of the  $i$ -th hole;  $\mathbf{H}$  is expressed in terms of scalar porosity  $p = (1/A)\pi \sum a^{(i)} b^{(i)}$  and a symmetric second rank tensor  $\boldsymbol{\beta} = (1/A)\pi \sum (a^2 \mathbf{nn} + b^2 \mathbf{mm})^{(i)}$ .

This establishes the basic framework for the analysis of various practically important distributions of shapes and orientations of pores. This work is currently underway.

REPORT DOCUMENTATION PAGE			Form Approved OMB No. 0704-0188	
<small>PUBLIC REPORTING BURDEN FOR THE COLLECTION OF INFORMATION IS ESTIMATED TO AVERAGE 1 HOUR PER RESPONSE, INCLUDING THE TIME FOR reviewing instructions, searching existing data sources, gathering and maintaining the data needed, and completing and reviewing the collection of information. Send comments regarding this burden estimate or any other aspect of this collection of information, including suggestions for reducing this burden, to Washington Headquarters Services, Directorate for Information Operations and Reports, 1215 Jefferson Davis Highway, Suite 1204, Arlington, VA 22202-4302, and to the Office of Management and Budget, Paperwork Reduction Project (0704-0188), Washington, DC 20503.</small>				
1. AGENCY USE ONLY (Leave blank)		2. REPORT DATE February 10, 1997	3. REPORT TYPE AND DATES COVERED Task 1 Report 11/7/96 - 2/6/97	
4. TITLE AND SUBTITLE CONTRACT NAS3-97002 "Heat Conduction in Ceramic Coatings: Relationship between Microstructure and Effective Thermal Conductivity"			5. FUNDING NUMBERS  WU-	
6. AUTHOR(S) Prof. Mark Kachanov				
7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES) Tufts University, Grants and Contracts Administration Attn: Theodore M. Liszczak Packard Hall, Room 103 Medford MA 02155			8. PERFORMING ORGANIZATION REPORT NUMBER  E-	
9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS(ES) National Aeronautics and Space Administration Lewis Research Center Cleveland, Ohio 44135 - 3191			10. SPONSORING/MONITORING AGENCY REPORT NUMBER  NASA CR-	
11. SUPPLEMENTARY NOTES				
12a. DISTRIBUTION/AVAILABILITY STATEMENT  Unclassified - Unlimited Subject Category			12b. DISTRIBUTION CODE	
13. ABSTRACT (Maximum 200 words)  <p>Research on the effective thermal conductivity of ceramic coatings and its relation to the microstructure continued. Experimental data on thermal conductivity of ceramic coatings provided by NASA (paper by R. Miller et al) indicates the necessity of construction a theoretical framework for the analysis of anisotropic conductivity in terms of the microstructural parameters. Our effort was focused on this task.</p> <p>We used the approach similar to the one developed earlier for elastic properties of materials with defects and developed it further for the thermal conductivity problem. We started with the analysis of the influence of one pore on the overall heat flux. This influence is strongly dependent on the shape of the pore. We model pores as insulators (this modelling can be viewed as the first approximation and can later be refined to account for a finite pore conductivity).</p> <p>We first analyzed pores of elliptical shapes. Such shapes, although simple, constitute an important example: they demonstrate the importance of shape factors. Also, they cover both cracks and circles as limiting cases, and allow one to consider the practically important case of mixtures of cracks/pores. We start with the analysis of an influence of one such pore on the overall heat flux and then analyze the case of many cracks in the non-interaction approximation.</p>				
14. SUBJECT TERMS			15. NUMBER OF PAGES 4	
			16. PRICE CODE	
17. SECURITY CLASSIFICATION OF REPORT Unclassified	18. SECURITY CLASSIFICATION OF THIS PAGE Unclassified	19. SECURITY CLASSIFICATION OF ABSTRACT Unclassified	20. LIMITATION OF ABSTRACT	